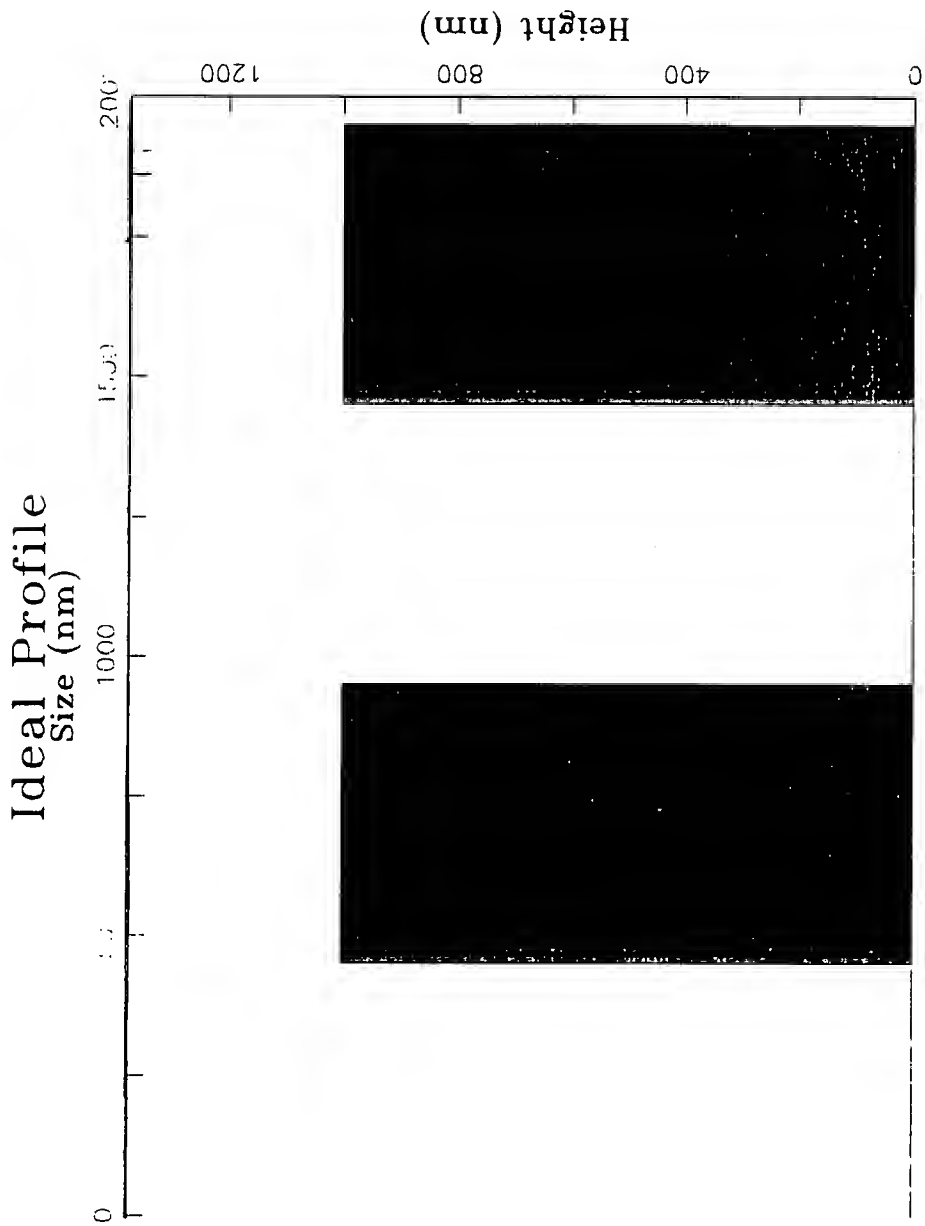


FIG. 2

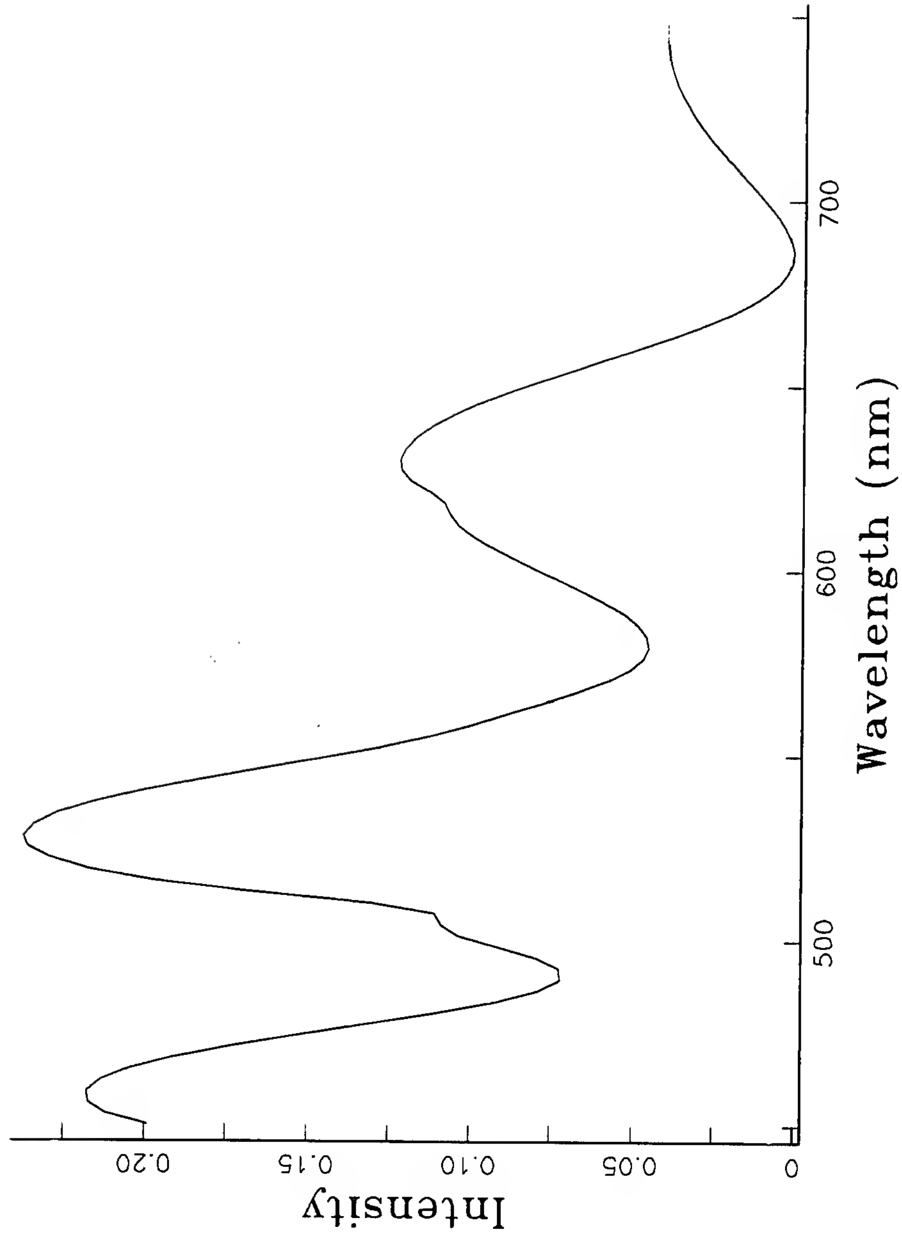


FIG. 3

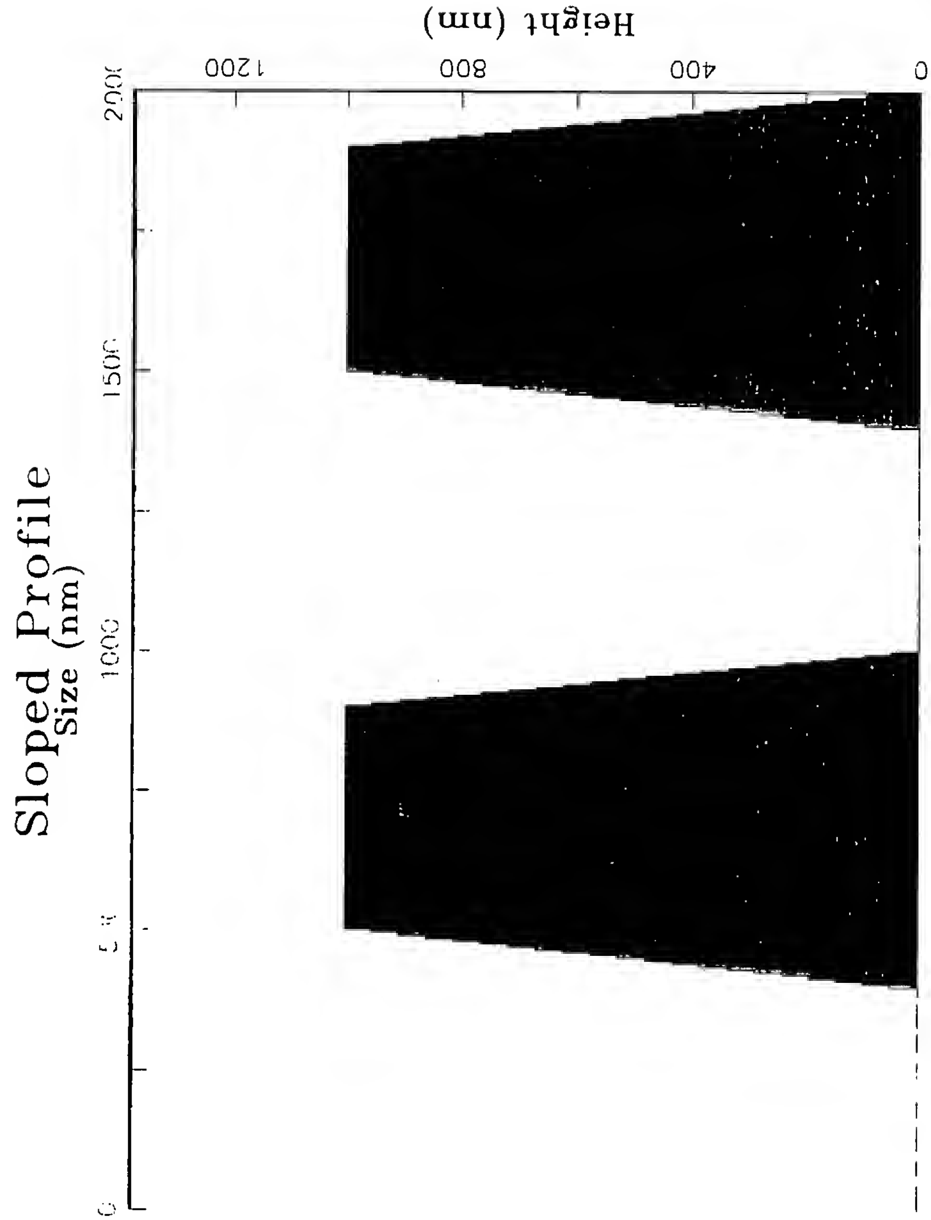

Sloped Profile
Height (nm)
0
400
800
1200
Size (nm)
0
500
1000
1500
2000

FIG. 4

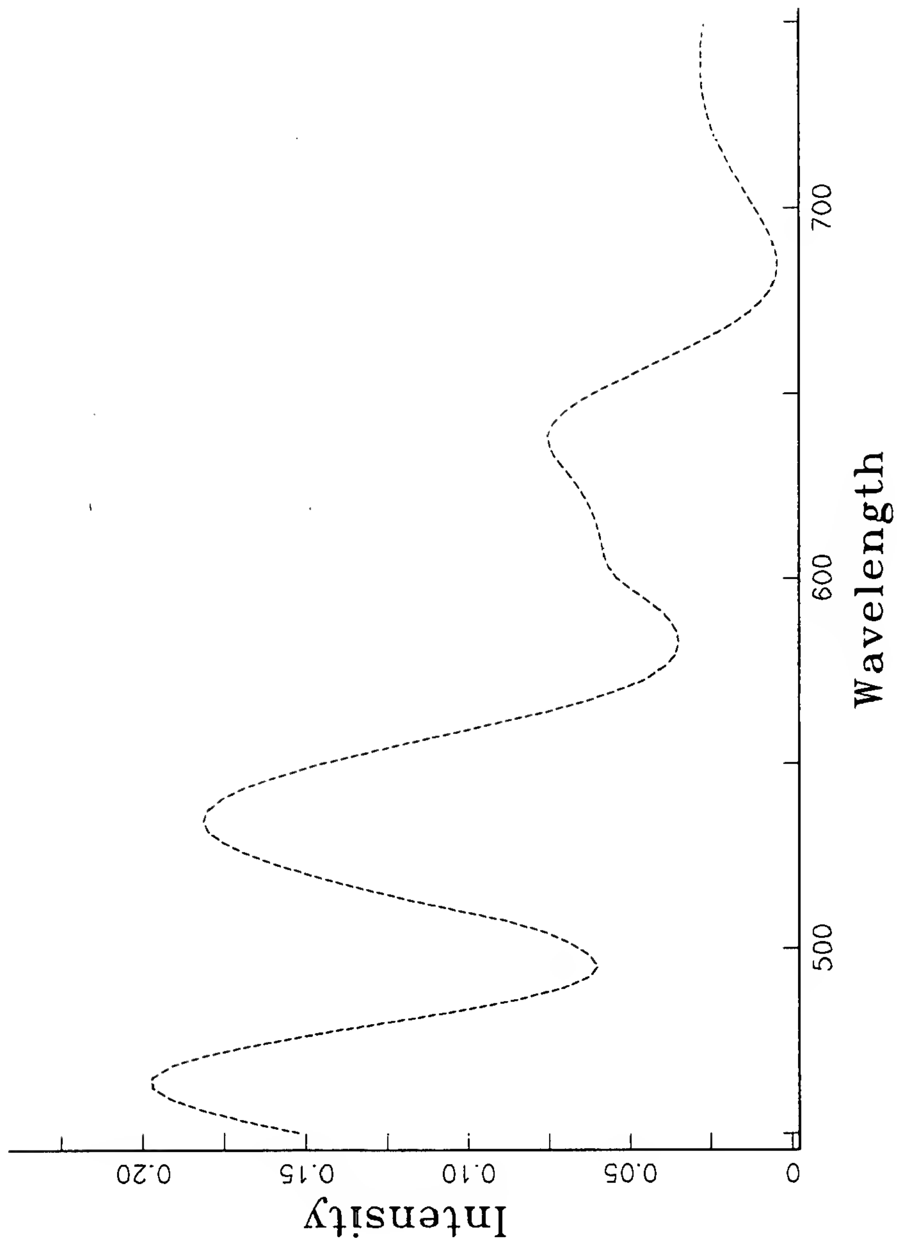


FIG. 5

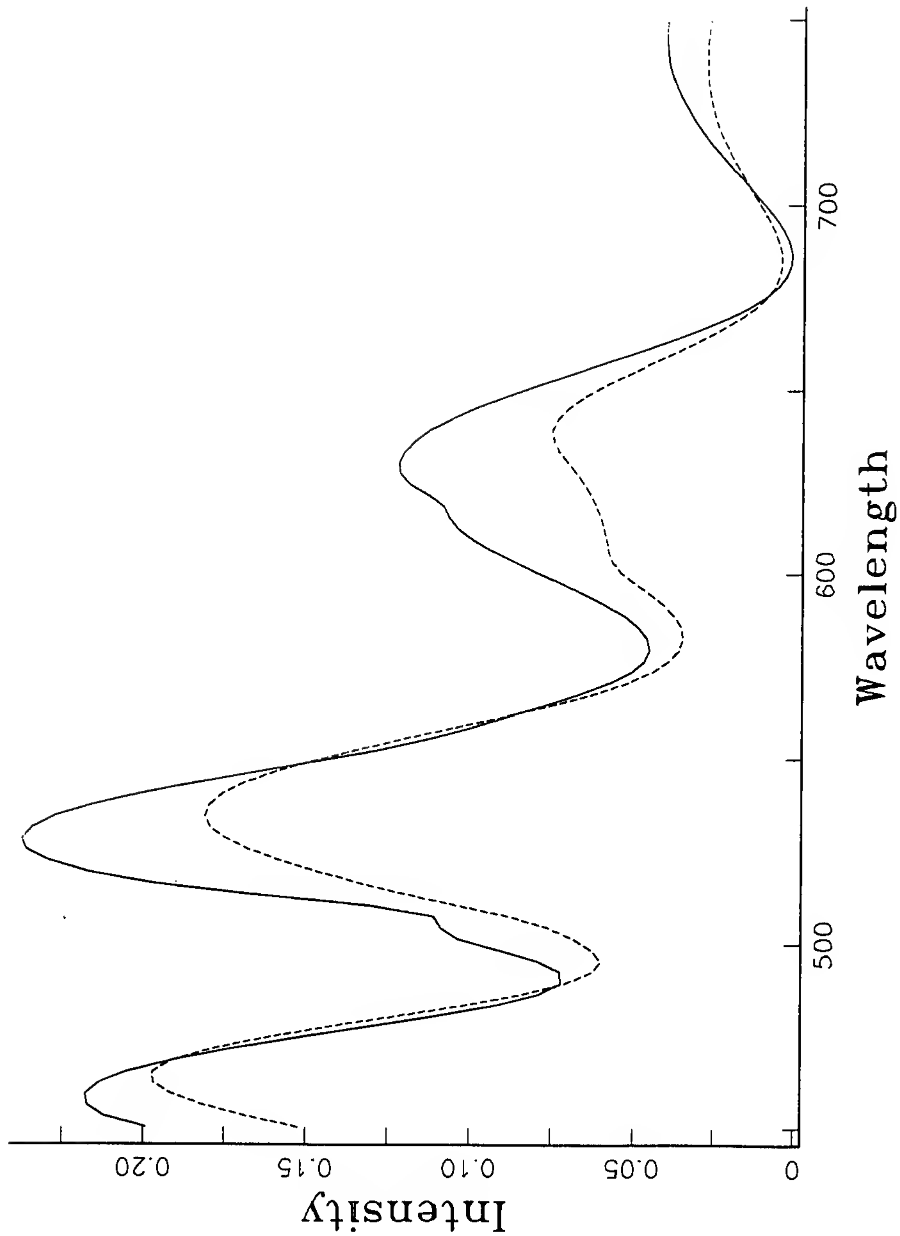


FIG. 6

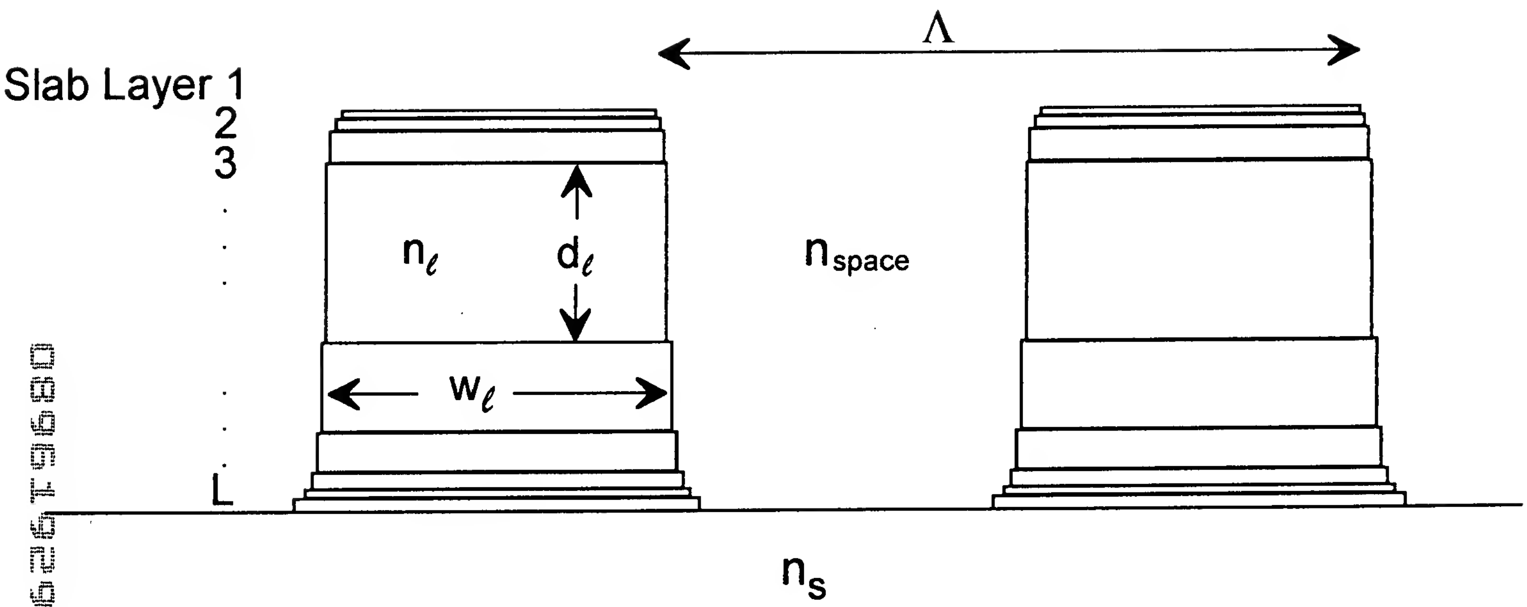


FIG. 7

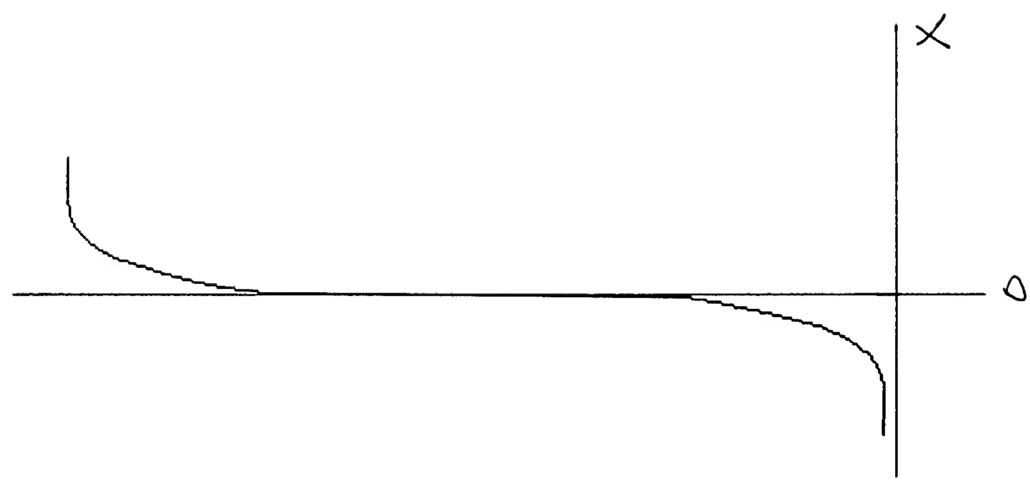


FIG. 8a

FIG. 8b

FIG. 8c

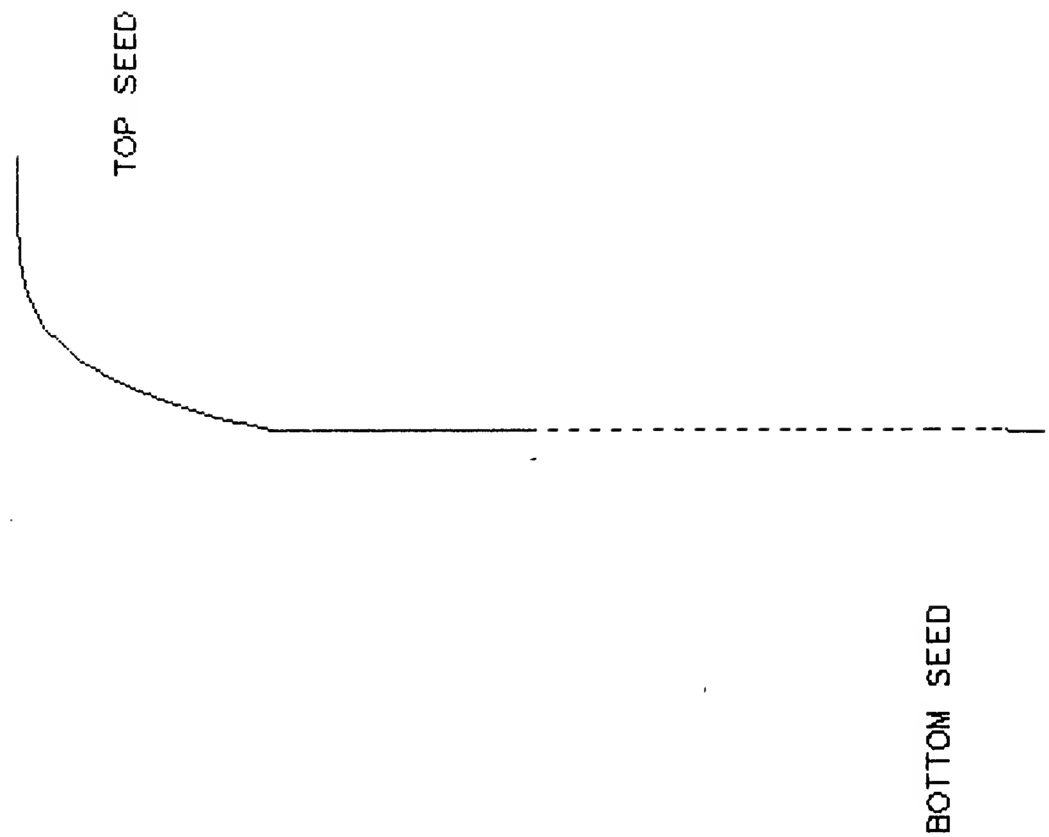


FIG. 8d

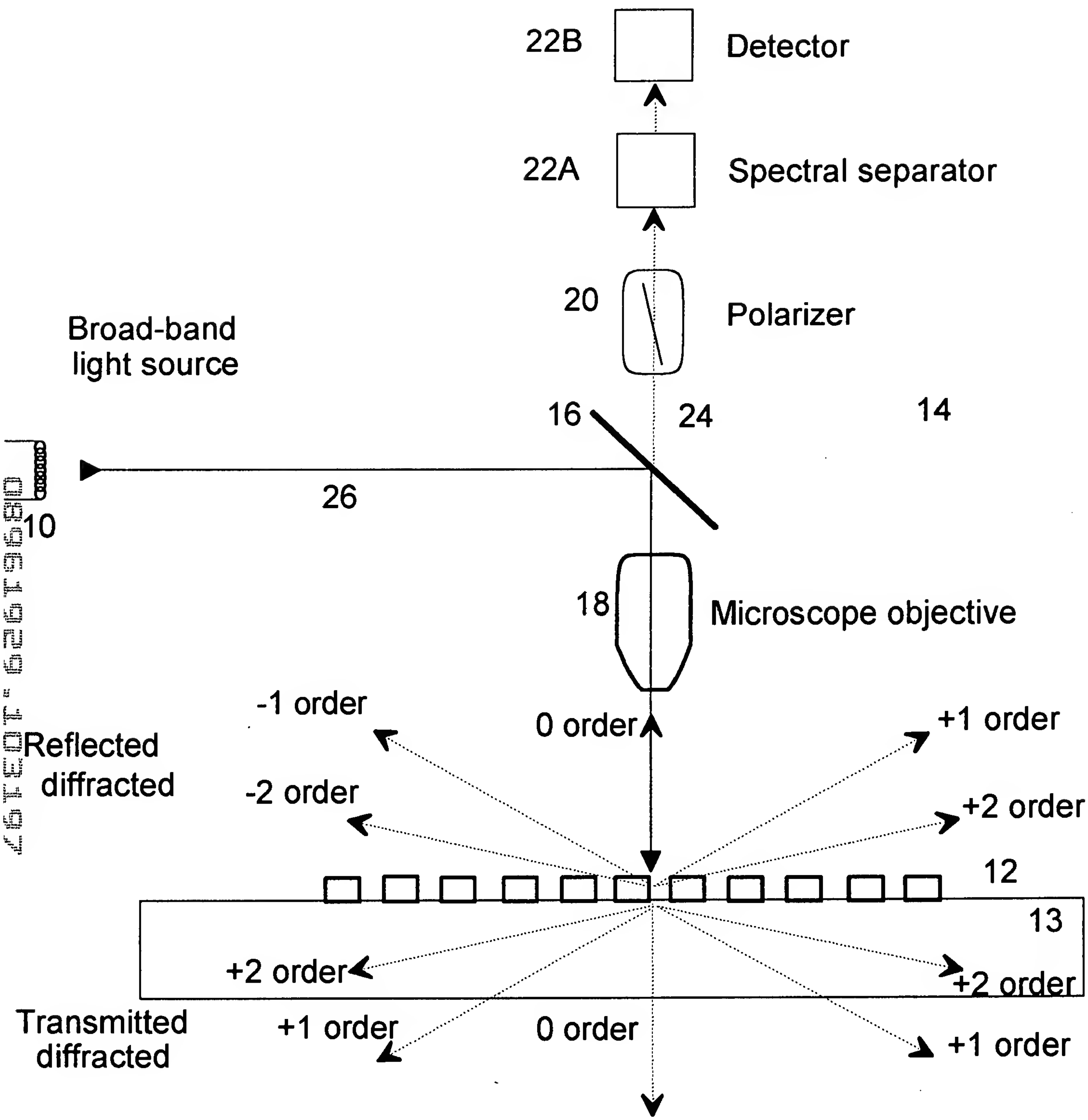

22B
Detector
22A
Spectral separator
20
Polarizer
Broad-band
light source
16
24
14
10
26
18
Microscope objective
-1 order
0 order
+1 order
Reflected
diffracted
-2 order
+2 order
12
13
+2 order
+2 order
Transmitted
diffracted
+1 order
0 order
+1 order

FIG. 9

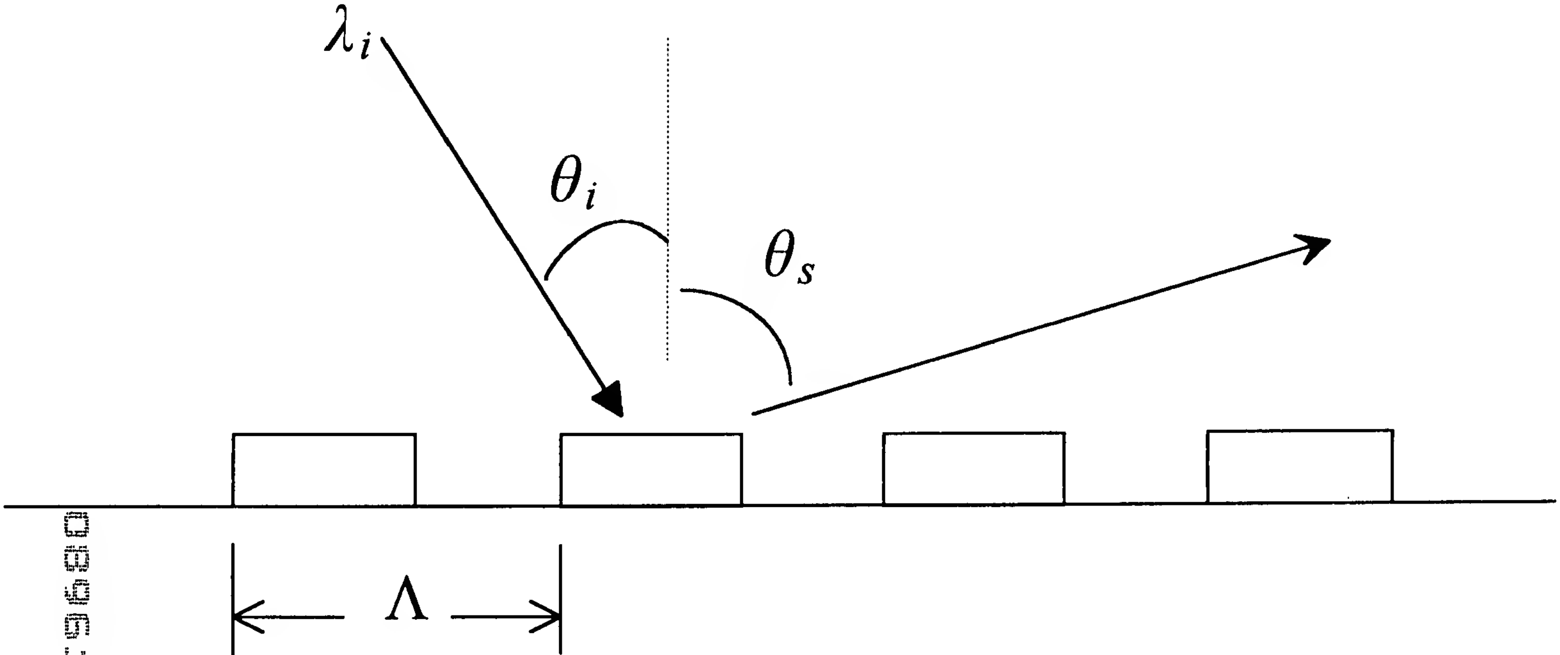


FIG. 10

FIG. 11

```
[0]   COUPLEDWAVE WL;TT;DD
[1]  ⍝  Set ORDERS = the number of +diffracted orders retained.
[2]   WAVELENGTH←WL
[3]   f←LAYER[;2]÷GRATINGPERIOD         ⍝ Determine f from dimensions
[4]   d←LAYER[;3]                       ⍝ Layer thicknesses
[5]   n0←1                              ⍝ Index of air
[6]   THETA←TH                          ⍝ Angle of incidence, degrees
[7]   THET←THETA×○1÷180                 ⍝ Incidence angle, radians
[8]   ns←SIINDEX WAVELENGTH             ⍝ Determine the substrate index
[9]   n←0⍴0
[10]  FILMINDEX¨LAYER[;1]               ⍝ Determine the FILM index
[11]  N←1+ORDERS×2                      ⍝ N will always be odd
[12]  h←(⍳N)-1                        : ⍝ h is  0 1 2 3 4 5 6 7...
[13]  i←h-((N-1)÷2)                     ⍝ i is  ...¯3 ¯2 ¯1 0 1 2 3...
[14] ⍝
[15]  I←,DD←(N,N)⍴0
[16]  TT←(N,N)⍴⍳N
[17]  I[(0=,(TT-⍉TT))/⍳N*2]←1
[18]  I←(⍴f)⍴⊂(⍴DD)⍴I                   ⍝ I is the identity matrix
[19]  IL←1⊃I
[20]  k0←○2÷WAVELENGTH
[21]  kxi←k0×(n0×1○THET) i×WAVELENGTH÷GRATINGPERIOD
[22]  k1zi←((-(TT<0)×2)+1)×(TT←((k0*2)×(n0*2))-(kxi*2))*.5
[23]  k2zi←(((k0*2)×(ns*2))-(kxi*2))*.5          ⍝ Absorbing substrate (Si)
[24] TM:
[25]  B←((K+.×¨(EE←⌹¨E←PERMITTIVITY))+.×¨K←WAVENUMBER)-¨I
[26] ⍝DERTM←0
[27] ⍝→TE
[28]  EIGENSTUFF E+.×¨B                 ⍝ TM eigenspace calculations
[29]  V←(EE+.×¨W)+.×¨Q                  ⍝ PRODUCT MATRIX FOR   TM  (EE IS ⌹¨E)
[30]  X←I×¨*-k0×¨Q×d                    ⍝ d SCALAR OR VECTOR WITH LENGTH OF f
[31]  DELTA←((2×N),1)⍴(i=0),((2○THET)×0J1÷n0)×i=0          ⍝ FOR TM
[32]  Z1←(1⊃I)×(N,N)⍴k1zi÷((n0*2)×k0)
[33]  Z2←(1⊃I)×(N,N)⍴k2zi÷((ns*2)×k0)
[34]  M1←IL,[1]-0J1×Z1
[35]  FG←(1⊃I),[1]0J1×Z2
[36]  FANDG¨⌽⍳⍴f
[37]  R←N↑,(-DELTA)⌹(M1,-FG)
[38] ⍝       Diffraction efficiency for TM
[39]  DERTM←(THETAOUT=TH)/(DERTM≠0)/DERTM←(R×+R)×9○(k1zi÷k0×n0×2○THET)
[40] ⍝ DERTM←(DERTM≠0)/DERTM←(R×+R)×9○(k1zi÷k0×n0×2○THET)
[41] ⍝
[42]  DERTE←0
[43]  →COMB
[44] TE:
[45]  A←(K+.×¨K)-¨E
[46]  EIGENSTUFF A                      ⍝ TE eigenspace calculations
[47]  V←W+.×Z¨Q                         ⍝ PRODUCT MATRIX FOR   TE
[48]  X←I×¨*-k0×¨Q×d                    ⍝ d SCALAR OR VECTOR WITH LENGTH OF f
[49]  DELTA←((2×N),1)⍴(i=0),((2○THET)×0J1×n0)×i=0          ⍝ FOR TE
[50]  Y1←(1⊃I)×(N,N)⍴k1zi÷k0
[51]  Y2←(1⊃I)×(N,N)⍴k2zi÷k0
[52]  M1←IL,[1]-0J1×Y1
[53]  FG←(1⊃I),[1]0J1×Y2
[54]  FANDG¨⌽⍳⍴f
[55]  R←N↑,(-DELTA)⌹(M1,-FG)
[56] ⍝           Diffraction efficiency for TE
[57]  DERTE←(THETAOUT=TH)/(DERTE≠0)/DERTE←(R×+R)×9○(k1zi÷k0×n0×2○THET)
[58] COMB:
[59]  CURVE←CURVE,[1]1 3⍴WAVELENGTH,DERTE,DERTM
```

FIG. 11(cont'd)

```
[60] ⍝CURVE←CURVE,[1]1 3⍴WAVELENGTH,DERTM,DERTE

[0]    EIGENSTUFF EI
[1]    Z←EIGEN¨EI           ⍝ The function EIGEN is an IBM program product
[2]    W←((⍴f)⍴⊂1 0)↓¨Z     ⍝   and cannot be shown here.
[3]    QQ←((⍴f)⍴⊂((-N),0))↓¨Z
[4]    Q←0⍴0
[5]    EIGENVALUE¨QQ
[6]    Q←Q×¨I

[0]    EIGENVALUE QQ
[1]    Q←Q,⊂(N,N)⍴QQ*.5

[0]    FANDG L;XA:XL;WL:VL
[1]    XL←L⊃X
[2]    WL←L⊃W
[3]    VL←L⊃V
[4]    AB←(⌹((-WL),[1]VL),FG)+.×(WL+.×XL),[1]VL+.×XL
[6]    A←(N,N)⍴AB
[7]    FG←(WL+.×IL+XA),[1]VL+.×IL-XA←XL+.×A

[0]    FILMINDEX FILM;C1;C2;C3;I
[1]    I←(20=+/¨((⊂FILM)=CAUCHY[;1]))/⍳1↑⍴CAUCHY
[2]    C1←CAUCHY[I;2]
[3]    C2←CAUCHY[I;3]
[4]    C3←CAUCHY[I;4]
[5]    n←n,C1+(C2÷(WAVELENGTH×10)*2)+C3÷(WAVELENGTH×10)*4

[0]    E←PERMITTIVITY
[1]    E←0⍴0
[2]    PERMPRIME¨⍳⍴f

[0]    PERMPRIME M
[1]    PP←(N,N)⍴h+1
[2]    II←⍉PP
[3]    EE←,((n[M]*2)-(n0*2))×(1○(○1×(II-PP)×f[M]))÷○1×II-PP
[4]    EE[(0=,(II-PP))/⍳N*2]←((n[M]*2)×f[M])+(n0*2)×(1-f[M])
[5]    E←E,⊂(⍴II)⍴EE

[0]    K←WAVENUMBER
[1]    K←(N,N)⍴k×i÷k0
[2]    K←(⊂K)×¨I

[0]    ns←SIINDEX WAVELENGTH:INDEX;A;ks
[1]  ⍝ Determine the complex refractive index from 210 to 825 nm.
[2]    INDEX←¯1+2↑(WAVELENGTH≤SI[;1])/⍳1↑⍴SI
[3]    ns←SI[INDEX[1];2]+(A←(WAVELENGTH-SI[INDEX[1];1])÷-/SI[INDEX;1])
×-/SI[INDEX;2]
[5]    ks←SI[INDEX[1];3]+A×-/SI[INDEX;3]
[6]    ns←ns-0J1×ks
```

The function COUPLEDWAVE is called by

COUPLEDWAVE WL

where WL is a required argument; its value being the wavelength at which to evaluate the theoretical profile. COUPLEDWAVE, as configured above, is set up to compute TM diffraction. To change to TE, remove the comment symbol from line 26 & 63 and add a comment to line 62. COUPLEDWAVE_also requires several other variables to be defined in the workspace:

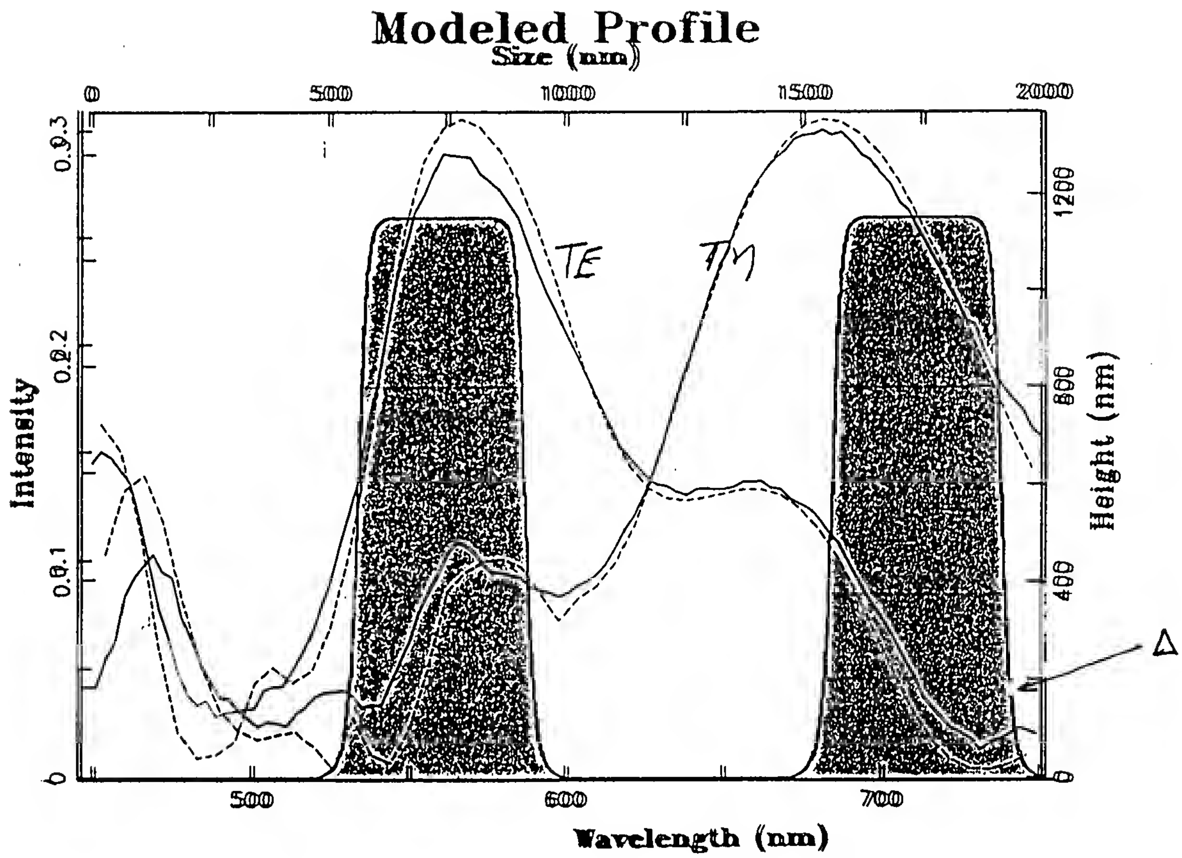
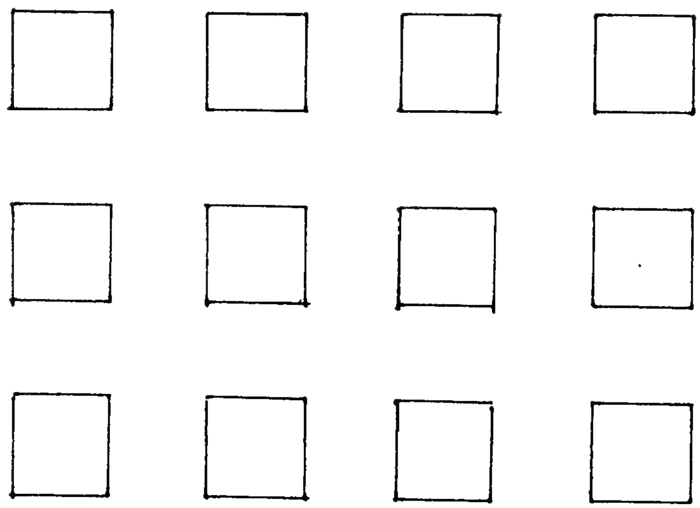

Modeled Profile
Size (nm)
0
500
1000
1500
2000
Intensity
0.3
0.2
0.1
0
Height (nm)
1200
800
400
0
500
600
700
Wavelength (nm)
TE
TM
Δ

FIG. 12

FIG. 13a



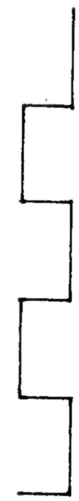


FIG. 13c

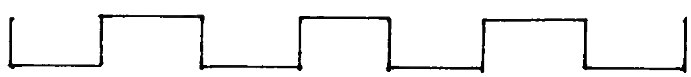


FIG. 13b

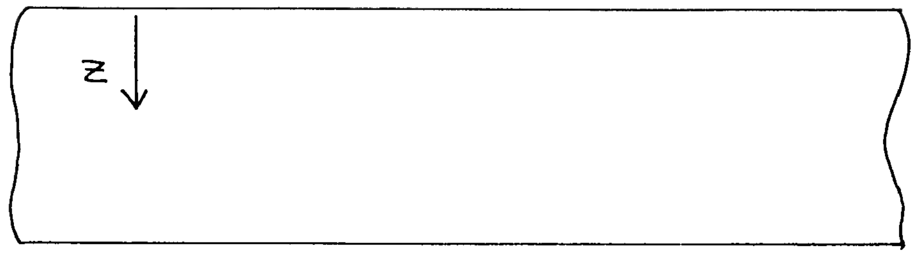


FIG. 14a

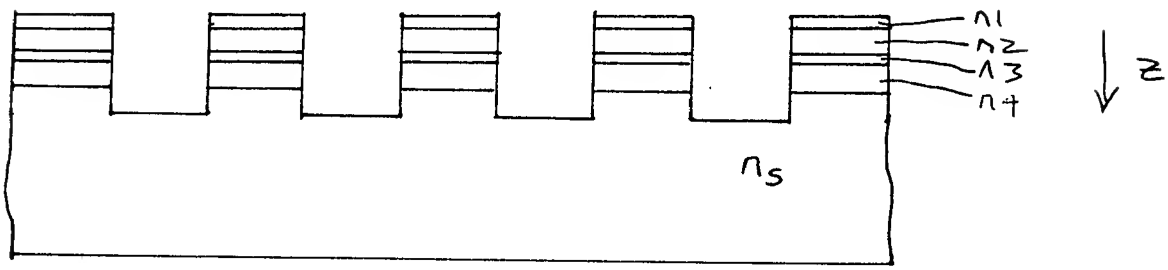


FIG. 14b

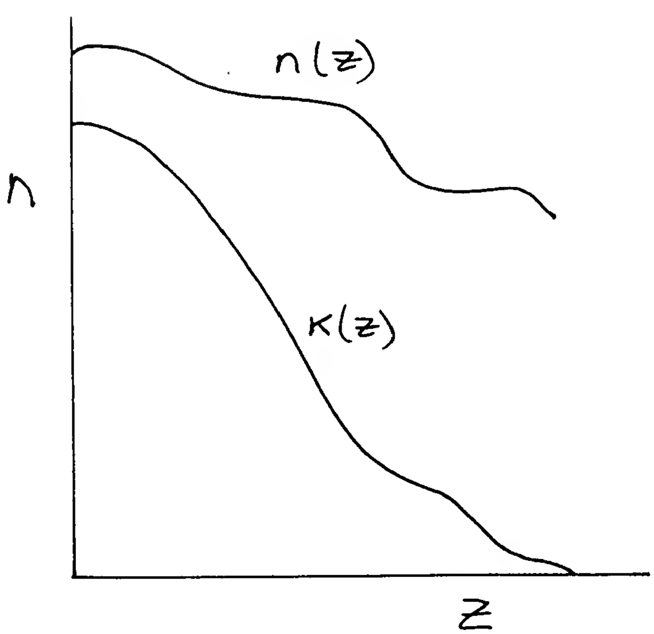


FIG. 14c

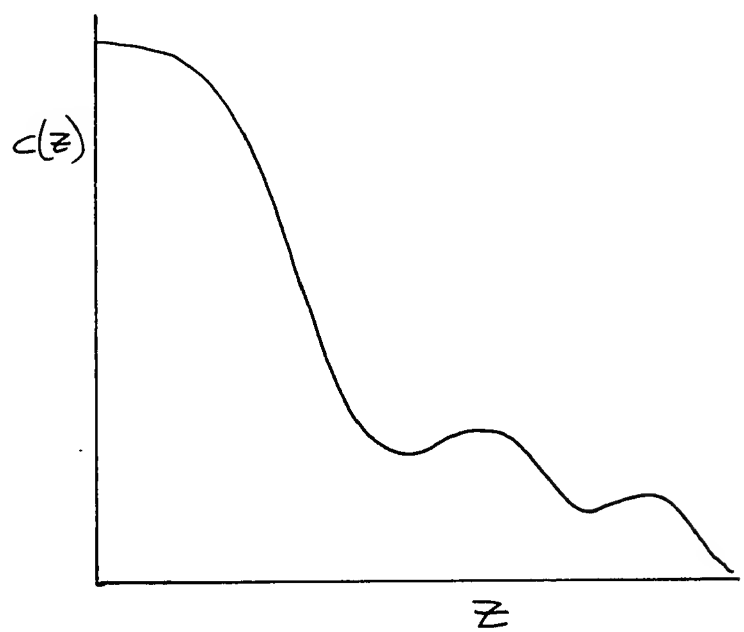


FIG. 14d

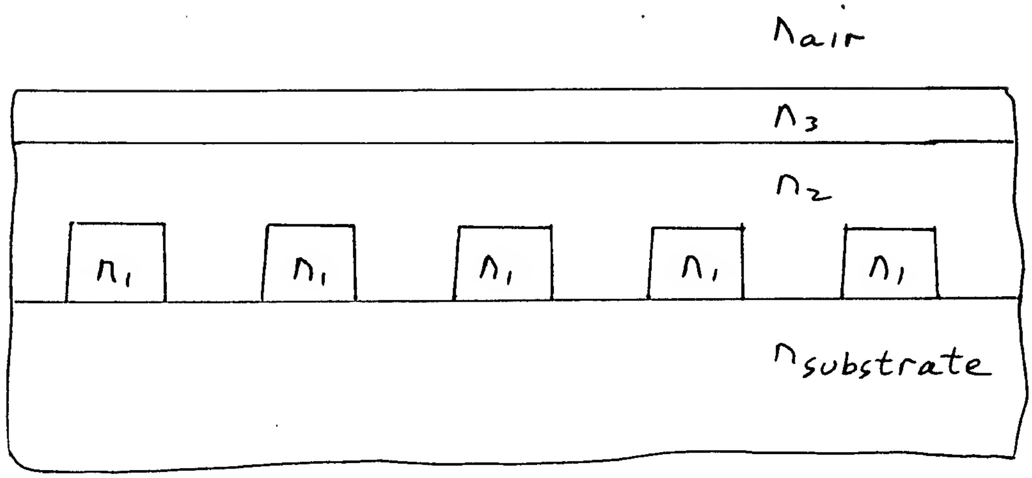


Fig. 15